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POTABLE WATER TASTE ENHANCEMENT

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to

The National Aeronautics and Space Administration

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## TABLE OF CONTENTS

1.0	INTRODUCTION. . . . .	1
2.0	LITERATURE FINDINGS . . . . .	3
2.1	General Principles of Taste and Odor . . . . .	3
2.2	Sources of Taste and Odor in Drinking Water. . . . .	4
2.3	Water Analysis Methods . . . . .	6
2.4	Water Standards. . . . .	7
2.5	Psychological Aspects in Water Quality Development . . . .	11
2.6	Palatability Related Factors . . . . .	12
3.0	EXPERIMENTAL APPROACHES . . . . .	16
3.1	Analytical Methods . . . . .	16
3.1.1	Inorganics, dissolved gases and organic carbon. . .	16
3.1.2	Qualitative volatile organic profiles . . . . .	17
3.1.3	Quantitation of volatile organics . . . . .	20
3.2	Preparation of Synthetic Water Samples for Taste Evaluation . . . . .	21
4.0	EXPERIMENTAL RESULTS AND DISCUSSION . . . . .	23
4.1	Evaluation of Waste Water Reclamation Systems. . . . .	23
4.1.1	Inorganic chemical constituents, dissolved gases, and organic carbon. . . . .	23
4.1.2	Volatile organic profiles . . . . .	25
4.2	Quantitation of Volatile Organics. . . . .	32
4.2.1	Discussion. . . . .	35
4.3	Taste Panel Evaluations. . . . .	44

## TABLE OF CONTENTS CONTINUED

5.0	CONCLUSIONS AND RECOMMENDATIONS . . . . .	50
5.1	Spacecraft Water Quality-Potability Specifications . . . .	50
5.2	Evaluation of Spacecraft Water Reclamation Systems . . . .	51
6.0	BIBLIOGRAPHY. . . . .	54
7.0	SUMMARY . . . . .	58
8.0	APPENDIX. . . . .	60
8.1	List of Figures. . . . .	60
8.2	List of Tables . . . . .	61

## 1.0 INTRODUCTION

Potable water used for manned spaceflight missions is characterized by an unpalatable flat or bitter taste because of contaminants and/or lack of specific ingredients. The absence of taste results from the removal of organic and inorganic compounds normally found in good tasting water supplies. Contaminants in spacecraft water systems which cause disagreeable taste may originate from several sources, including improper cleaning, leaching from incompatible materials, and inefficient removal with subsequent build-up of certain components in recycling systems. The unpalatability of spacecraft potable water dictates the need to (a) establish criteria for the enhancement of taste of purified water; (b) identify contaminants causing disagreeable taste and determine ways of removing them; and (c) evaluate and develop techniques for monitoring and maintaining water quality and palatability. It was intended that the effort under this contract utilize to the fullest extent any applicable information available in the published literature to accomplish (a), (b) and (c) above.

The principal objectives during the first year effort were, therefore, (i) to conduct a comprehensive literature search on the effects of various common water constituents on palatability and the evolution of analytical methods for determining these constituents; (ii) to develop preliminary criteria and specifications for palatable water to serve as guidelines for subsequent phases of investigation; and (iii) to perform laboratory analyses of selected water samples for preliminary evaluation of reclaimed water samples and measurement of chemical constituents related to palatability.

The results of the first year's effort indicated that the total quantity of volatile organics present in spacecraft water must be maintained at some value in the 10-1,000 ppb (parts per billion) range to insure against possible negative palatability effects. Single component concentrations may have to be controlled to lower concentrations depending on the particular component. It was apparent that any further definition of the volatile organics specification would require quantitative data on volatile organics in potable water. The literature search indicated that no published methods were available for these determinations. A considerable portion of the final year effort was, therefore, devoted to the development of a technique for the quantitative analysis of volatile organics in water. The remaining effort was devoted to the further examination of the palatability factors developed during the first year in an attempt to determine which are actually essential for good tasting water.

## 2.0 LITERATURE FINDINGS

### 2.1 General Principles of Taste and Odor

There are many factors governing the taste and odor sensations and a fairly complete discussion requires several hundred pages. There are several factors which would seem to be more important in relation to water palatability. Probably the single most important factor is that, while taste and odor are separate, it is very difficult to dissociate them. This can be demonstrated by the fact that apparently tasty substances are tasteless when the nose is held. For this reason one must consider both taste and odor in discussions of palatability.

Both taste and odor have some fairly specific relations to chemical constituents which have been described in the literature (1-4). Tastes, however, are few and well-defined, while odors are ill-defined and subjective in nature. For the most part (but not conclusively) tastes can be classified as salty, sour, sweet and bitter. Sapid or tasteful substances are in a different class altogether than odorous substances. Substances which have the strongest tastes, such as polyhydric alcohols, sugars, amides, imides, salts and many mineral acids are odorless. In general, there appear to be two prerequisites for taste; (1) water solubility and (2) a molecular configuration which finds its complement in the taste receptors. Correspondingly, the prerequisites for odor appear to be (1) volatility and (2) a molecular configuration complementary to one that occurs in the olfactory receptors. The principle difference then is that taste requires water solubility while odor requires volatility. It should also be noted that stimulus of gustation or taste requires parts per million

concentrations in a few cc of water ( $10^{-6}$  g quantities); while stimulus of olfaction requires  $10^5$ - $10^6$  molecules per second for a few seconds ( $10^{-14}$  g quantities). Based on the above it would appear that volatile organic compounds amenable to analysis by head space sampling techniques may be important in determining water palatability.

## 2.2 Sources of Taste and Odor in Drinking Water

Several books have been published which treat the problem of taste and odor in drinking water with varying degrees of completeness. It should be noted, however, that in nearly all these publications the topic is approached from the negative standpoint; that is, what made the water taste or smell bad. This is even more pronounced in the case of organic constituents. Also, the analytical methods used to identify organic constituents are generally quite crude, the instrumentation often being a "chemist's" nose.

Some authorities state that "public water supplies should be of such palatability that they produce no sensation of either taste or odor." (2) This philosophy is not agreeable with our findings especially for spacecraft use, and furthermore, the absence of any taste and/or odor does, in fact, render the water less palatable. It is noted that it is possible for waters to possess taste without odor even though the presence of odors always gives rise to complaints of taste. Tastes without odor are usually due to the presence of certain mineral or saline constituents. NaCl and  $\text{Na}_2\text{SO}_4$  impart saline taste. Fe, Mn, Zn, excess of free lime  $\text{Ca}(\text{OH})_2$ , and Al compounds produce an astringent (equated to bitter or metallic) taste. Cu in excess of 1 ppm may impart a disagreeable taste.

The temperature of the water will have a pronounced effect on palatability, since both solubility and volatility are strong functions of temperature.

Certain waters also have an action on the palate which could not be described as either taste or odor. Chalk-derived waters, for example, are reported to possess a "sharpness" or pleasant palatability, probably due to the presence of  $\text{CO}_2$  and  $\text{CaHCO}_3$ . On the other hand, waters derived from surface sources and waters which are very soft or are deficient in oxygen are often described as flat or insipid. This would indicate dissolved gases play an important role in palatability. Organic contamination in public water supplies produces tastes and odors described as musty, earthy, weedy or moldy. Algae, protozoa, actinomycetes and other microorganisms produce tastes and odors described as musty, earthy, fishy, aromatic, etc. and are often accentuated by chlorine. One author states the most palatable waters are those containing nitrates and free  $\text{CO}_2$ , even though they may have been derived by degradation of objectionable microorganisms.

In summary it can be stated that the presence of taste and odor in water supplies is due to one or a combination of the following:

- (1) Presence of dissolved gases ( $\text{H}_2\text{S}$ ,  $\text{CO}_2$ ,  $\text{O}_2$ , etc.)
- (2) Contamination by contact with improperly prepared surfaces
- (3) Contamination by organic matter from sewage, manure, soil and vegetation
- (4) Contamination by chemicals such as industrial wastes
- (5) Growth of algae, protozoa, fungi, etc.
- (6) Treatment processes applied, e.g., chlorination, filtration, etc.



### 2.3 Water Analysis Methods

Our interest in water analysis methods was threefold. First, we wanted to select the best methods for subsequent analysis of palatability. Secondly, we wanted to evaluate methods for their potential in spacecraft water quality monitoring; and finally, we hoped that the literature would have mentioned palatability even though it did not appear in key phrases. (About twenty papers on water regenerating systems were also read with the latter in mind). We were particularly interested in organic compounds, both volatile and nonvolatile. Thirty-one papers were examined of which two were general reviews and are listed in the bibliography (5-30). The most pertinent of these is the review (6) published in Analytical Chemistry in 1971 which covers the following constituents: Alkali metals; Al, Fe, Mn, Cr, Os, and Re; Cu, Zn, Pb, Cd, Ni, Co, Ge, and In; Hg, Ag and Au; Va, Zi, Wg, Mo, Sc, U, and rare earths;  $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ; B, Se, As and Sb; fluoride; phosphorous and silica; nitrate, nitrite and nitrogen compounds; pH and alkalinity; oxygen demand; oxygen and other dissolved gases; detergents, pesticides and herbicides; organics; and radioactivity and isotopic analysis. With the exception of the organics, the methods reviewed are adequate for all constituents that may be of importance in palatability considerations. The methods cited for organic compounds are for dissolved material in microgram quantities and, therefore, are not sufficiently sensitive (odor sensations are produced by  $10^{-14}$  g quantities).

Several of these papers (15-30) deal with the analysis of headspace volatiles above pure compounds, aqueous solutions and foods, and volatile organics in room air. These methods were of interest to compare to our

proposed headspace analysis technique for organic volatiles in water.

The methods found in the literature exhibited one or more of the following deficiencies: (1) low sensitivity because of lack of any concentration step, (2) requiring analysis times of 24-72 hours, and (3) incomplete separation of the complex organic mixture contained in the sample.

#### 2.4 Water Standards

Water quality standards have been developed over the years for public drinking water with the primary purpose of minimizing toxicity problems which could arise in uncontrolled water supplies. Secondary considerations have included a desire to produce an attractive (equated to colorless) and palatable (no undesirable taste or odor) water so as to discourage the use by the public of other water supplies which are not safe. In the past fifteen years many different types of engineering devices have been developed in the space program to produce water from human waste, chamber atmosphere, and  $O_2-H_2$  fuel cells. This has led to the generation of a set of aerospace potable water standards which in some degree take into account the special problems associated with reclaimed water. Table 1 lists the International, USPHS, American Water Works Association, and recommended (Slonim et al, 1967) aerospace water standards for comparison purposes. The aerospace water standards are higher values in general for chemical constituents which can be justified by the short (compared to a normal life span) exposure to such water. It is possible that many of these chemicals could be eliminated from spacecraft water potability criteria if certain materials are not present in the spacecraft water system, and thereby eliminate many monitoring requirements. On the

TABLE 1  
Comparison of Water Standards

Water Quality Criteria	International	Public Health Service	AWWA <sup>(1)</sup>	Aerospace
<u>BIOLOGICAL</u>				
Coliform organisms/100 ml	10 <sup>(2)</sup> ; 1.0 <sup>(3)</sup>	1.0	0.1	None
Coliform organisms, total count	No limit	No requirement	No requirement	None
Micro organisms	No requirement	No requirement	0	200/ml
Viruses	No requirement	No requirement	No requirement	No requirement
<u>PHYSICAL</u>				
Color, cobalt scale units	5	15	3	15
Odor (threshold no.)	Unobjectionable	Inoffensive <sup>(4)</sup>	No requirement	3
Taste (threshold no.)	Unobjectionable	Inoffensive	None	3
Turbidity, silica scale units	5	5	0.1	25
<u>CHEMICAL</u> <sup>(5)</sup>				
Alkyl benzene sulfonate	0.5	0.5 <sup>(6)</sup>	0.2	None
Aluminum	No requirement	No requirement	0.05	No requirement
Arsenic	0.05	0.01 <sup>(6)</sup> 0.05 <sup>(7)</sup>	0.01	0.5
Barium	1.0 <sup>(8)</sup>	1.0 <sup>(7)</sup>	0.5	2.0

TABLE 1 (CONT'D)

-2-

Water Quality Criteria	International	Public Health Service	AWWA <sup>(1)</sup>	Aerospace
<u>CHEMICAL</u> <sup>5</sup> (cont'd)				
Cadmium	0.01 <sup>(8)</sup>	0.01 <sup>(7)</sup>	0.01	0.05
Calcium	75	No requirement	No requirement	No requirement
Calcium carbonate <sup>(9)</sup>	No requirement	No requirement	86	No requirement
Carbon alcohol extract	No requirement	No requirement	0.1	No requirement
Carbon chloroform ex.	0.2	0.2 <sup>(6)</sup>	0.04	100 <sup>(13)</sup>
Chloride	200	250 <sup>6</sup>	No requirement	450
Chromium, hexavalent	0.05 <sup>(8)</sup>	0.05 <sup>(7)</sup>	0.01	0.05
Copper	1.0	1.0 <sup>(7)</sup>	0.2	3.0
Cyanide	0.2 <sup>(8)</sup>	0.01 <sup>(6)</sup> 0.2 <sup>(7)</sup>	0.01	No requirement
Fluoride	1.0-1.5	0.8-1.7 1.4-2.4	0.7-1.2	2.0
Hydrogen ion (pH)	7.0-8.5	No requirement	No requirement	5.0-10.0
Iron	0.3	0.3 <sup>(6)</sup>	0.05	1.0
Lead	0.05 <sup>(8)</sup>	0.05 <sup>(7)</sup>	0.05	0.2
Magnesium	50	No requirement	No requirement	No requirement
Magnesium + sodium sulfate	500	No requirement	No requirement	No requirement
Manganese	0.1	0.05 <sup>(6)</sup>	0.01	0.1
Nitrate	45	45	23	100
Phenol	0.001	0.001 <sup>(6)</sup>	0.0005	0.05
Selenium	0.01 <sup>(8)</sup>	0.01 <sup>7</sup>	0.1	0.05
Silver	No requirement	0.05 <sup>7</sup>	0.02	0.5
Sulfate	200	250	No requirement	250
Zinc	5.0	5.0 <sup>(6)</sup>	1.0	15
Total dissolved solids	500	500	No requirement	1000 <sup>(12)</sup>

TABLE 1 (CONT'D)

-3-

Water Quality Criteria	International	Public Health Service	AWWA <sup>(1)</sup>	Aerospace
<u>RADIOCHEMICAL</u>				
Strontium-90	30	10 <sup>(11)</sup>	5	10
Radium-226	10	3 <sup>(11)</sup>	3	3
Gross beta	1000	1000 <sup>(11)</sup>	100	1000
Reference	(C)	(B)	(A)	(D)

REFERENCES AND FOOTNOTES

- (A) American Water Works Association. 1967. Willing Water 11(6).
- (B) U.S. Public Health Service. 1962. U.S. Public Health Service P. 956
- (C) World Health Organization. 1963. International standards for drinking water. Columbia University Press: New York.
- (D) Slonim, A. J. et al, Aerospace Medicine, 38, pp. 793-799, 1967.  
1. Criteria are tentative. 2. In 90% of the samples untreated water examined in any one year. 3. In treated water. 4. Maximum threshold number, 3. 5. Values are ppm, except the value for pH. 6. Recommended. 7. Mandatory limit. 8. Tolerance limit, comparable to the mandatory limit of the Public Health Service standards. 9. Criterion for hardness. 10. Values are c/liter. 11. For full interpretation, consult 1962 Public Health Service Drinking-Water Standards. 12. Total solids. 13. Chemical oxygen demand-COD.

other hand, certain constituents might have to be added because of the nature of the system.

Although the aerospace standards in Table 1 contain limits for taste, odor, phenol, dissolved solids, and micro-organisms, they do not adequately consider palatability and are primarily based on toxicity. Phenolic compounds are present infrequently and have probably been overemphasized because they are one of the few materials detectable by analytical techniques generally available in water plant laboratories. Before chlorination, commonly occurring phenolic materials have little taste or odor. Other treatments can destroy the odor. The inclusion of values for dissolved gases deserves careful consideration. Furthermore, one can index organic content in several ways: BOD, COD, DOC (dissolved organic carbon), organic nitrogen, etc. are examples of group methods. This group treatment, however, is not sufficient for palatability considerations and individual taste and odor producing components indices must be derived. These individual components will be those known to be associated with a particular water supply (whether it be storage or regenerative), which also cause a significant organoleptic response.

## 2.5 Psychological Aspects in Water Quality Development

<sup>A</sup>In a concept of regenerated water quality development, the establishment of potability and palatability criteria must be reviewed in terms of psychological barriers toward consumer acceptance. The consumers' awareness of the technologies involved in the production of the product water is as significant as the maintenance of qualities such as odor, taste, turbidity, toxicity, etc. It is, then, important in the development of new

methods of closed-ecological water regenerating systems that a simultaneous educational effort be undertaken in order to overcome obvious psychological barriers for acceptance. Educating the user in the principles of hydro-chemistry and the reclaiming process can be helpful. The increased effort required to monitor the physical, chemical, and biological properties of the regenerated water should also be pointed out.

## 2.6 Palatability Related Factors

General considerations for potable and palatable water include (a) toxicity; (b) mineral constituents, dissolved gases, dissolved (nonvolatile) organic compounds, and volatile organic compounds affecting taste and/or odor; (c) color producing material; (d) total solids; (e) psychological factors; and (f) physiological factors. Specifications for inorganic and organic components related to toxicity considerations may (1) exclude or reduce the amount of those in USPHS criteria because of short exposure (e.g., As, Ba, Cd, Cr, F, Pb, Zn, Mn, Se) (2) add additional components or amounts because of the peculiarities of the particular storage or regenerative system supply (e.g., Be, B, Hg, V, Sb, Cs, I, Li, Pt and unknown urine volatile organics).

Our laboratory investigations and many of the references in the bibliography (11-15, 25, 27, 28, 30, 31) make it clear that extremely small amounts of odorous materials can cause sensory stimulation. Experiments have frequently yielded a detectable odor from recovered materials in concentration of 2 ppb and less. Sometimes materials have been isolated which could be detected by odor in concentrations less than 0.01 ppb. Utilizing adsorption and extraction techniques for concentrating odorous

organic constituents of drinking water supplies, it has been found that neutral compounds are usually the most abundant odorous organics present. These neutral organic materials usually have intense tastes and odors. The second most abundant group of odorous materials is usually the organic acids, which also have intense odors and tastes. Small quantities of other materials have been recovered, including organic bases (which may have a tobacco-like odor), water soluble compounds (which frequently have a caramel-like odor), and a group usually referred to as the weak acids which include phenolic compounds, if they are present in water.

The references to palatability found in the literature are generally negative. That is, chemical constituents which give rise only to undesirable tastes and odors are described. Table 2 summarizes the negative and positive (enhancement) factors related to palatability. Many other anions, cations, and dissolved gases are known to have negative effects on palatability, but those listed are most often encountered.

Based on the above, the first consideration in the production of taste enhanced potable water is the removal of all mineral constituents, volatile odor compounds, color producing material and microorganisms. Various methods are available including ion exchange, membrane filtering, vapor pyrolysis, and distillation; but the starting material should be equivalent to a quadruply distilled water. Taste producing compounds can then be added to the water to give the desired taste enhancement.

The taste of water is affected by the common dissolved minerals: calcium, magnesium, potassium, sodium, bicarbonate, carbonate, chloride, fluoride, nitrate, and sulfate. Complete removal of these minerals



TABLE 2

## PALATABILITY RELATED FACTORS

NEGATIVE FACTORSINORGANIC ANIONS AND CATIONS

$\text{NaCl}$ ,  $\text{Na}_2\text{SO}_4$   $\longrightarrow$  SALTY TASTE  $> 250$  PPM

$\text{Fe}$ ,  $\text{Mn}$ ,  $\text{Zn}$ ,  $\text{Ca}(\text{OH})_2$ ,  $\text{Al}$   $\longrightarrow$  BITTER OR METALLIC TASTE 10-50 PPM

$\text{Cu}$   $\longrightarrow$  DISAGREEABLE TASTE 1 PPM

DISSOLVED GASES

AMMONIA ( $\text{NH}_3$ ) AND HYDROGEN SULFIDE ( $\text{H}_2\text{S}$ )

ORGANIC COMPOUNDS

CERTAIN ACIDS, IMIDES, AMIDES, AMINES, PHENOLS

BUT NO INFORMATION ON VOLATILE ORGANICS

ENHANCEMENT FACTORS

$\text{Ca}^{++}$ ,  $\text{Mg}^{++}$ ,  $\text{K}^+$ ,  $\text{Na}^+$

$\text{HCO}_3^-$ ,  $\text{CO}_3^{--}$ ,  $\text{Cl}^-$ ,  $\text{F}^-$ ,  $\text{NO}_3^-$ ,  $\text{SO}_4^{--}$

$\text{O}_2$ ,  $\text{CO}_2$  AND PERHAPS  $\text{N}_2$

SOME ALCOHOLS, ACIDS, AND SUGARS BUT

NOTHING REPORTED ON VOLATILE COMPOUNDS

produces a flat, bitter tasting water. A certain amount of each of these minerals should be added back to produce a water with approximately 100 to 150 ppm total dissolved solids. A Russian worker (44) has also observed a possible negative physiological reaction in human subjects consuming water lacking these chemical components, (especially calcium and fluoride), but otherwise on a normal diet. This would indicate there are also physiological reasons for adding back these minerals. The optimum concentration of these minerals can only be determined by detailed taste panel evaluations of chemically analyzed test waters.

It appears that dissolved gases ( $O_2$ ,  $CO_2$  and perhaps  $N_2$ ) should also be added back to the water. It is difficult to estimate values at this time, but the range 1-5 ppm  $O_2$  found in natural waters can be a starting point. Final values here again must be determined by taste trials.

### 3.0 EXPERIMENTAL APPROACH

Several water samples, including product waters from prototype water reclamation systems, were evaluated for taste and chemically analyzed for the constituents listed in Table 2 which were those deemed most essential for good tasting potable water. This included analyses for anions, cations, acidity, pH,  $\text{NH}_3$ , dissolved gases, total organic carbon, particulate organic carbon, dissolved organic carbon, and volatile organic qualitative profiles. The procedures used for these analyses are described in the analytical methods section.

The quantification of individual volatile organic components was attempted utilizing the same solid adsorbent trapping and analysis technique used for qualitative volatile organic profiles. The technique was modified somewhat to optimize quantification of nanogram amounts. Methods of preparing standards and a description of the detailed quantitative procedures are given.

Synthetic water samples were fabricated by adding chemicals to specially prepared ultraclean water for palatability tests by a taste panel. Preparation of these samples and procedures for tasting are described.

#### 3.1 Analytical Methods

##### 3.1.1 Inorganic, Dissolved Gases and Organic Carbon

Reference to the 13th Edition (1971), Standard Methods for the Examination of Water and Wastewater is made for the following: dissolved  $\text{CO}_2$ , sulfates, ammonia -  $\text{N}_2$  and fluorides. A Fisher pH meter was used for pH measurements; dissolved oxygen was determined on a

Weston-Stack Analyser and a Beckman Carbonaceous Analyser was used for total organic carbon, particulate organic carbon, dissolved organic carbon and total inorganic carbon.  $\text{Ca}^{++}$ ,  $\text{Mg}^{++}$ ,  $\text{K}^+$ , and  $\text{Na}^+$  were run by atomic absorption spectroscopy according to the procedures in Water Analysis by Atomic Absorption Spectroscopy, by C. R. Parker, Varian Techon Pty. Ltd. Springvale, Australia (1972).

### 3.1.2 Qualitative Volatile Organic Profiles

Volatile organic compounds in the water samples were collected on a solid adsorbent trap by a headspace sampling technique. Figure 1 shows a cross sectional view of the trap and the modified gas chromatograph injector port which is used to desorb the trap. The adsorbent was Tenax GC 35/60 mesh (supplied by Applied Sciences, Inc., State College, PA). Figure 2A shows a diagram of the sampling apparatus. The liquid is placed in a 100°C water bath and the headspace swept with helium at 20 ml/min for approximately one hour. Sample sizes of 200 ml were extracted in this manner. Volatilization was increased by the addition of  $(\text{NH}_4)_2\text{SO}_4$  (30% w/v). The trapped sample was then stored in a clean teflon lined screw cap sealed Pyrex vial for subsequent analysis. The purge gas and volatiles are passed through a short water condenser prior to introduction to the adsorbent trap.

The analysis was begun by removing the trap from the storage tube and inserting it into the modified injector port (Figure 1) of a Perkin-Elmer 900 gas chromatograph. The sample was thermally desorbed for 20 minutes into a dry ice cooled capillary pre column (10' x .02" i.d.) (Figure 2B). After the allotted transfer time, the coolant was removed

FIGURE 1

TEXAX TRAP AND INJECTOR PORT

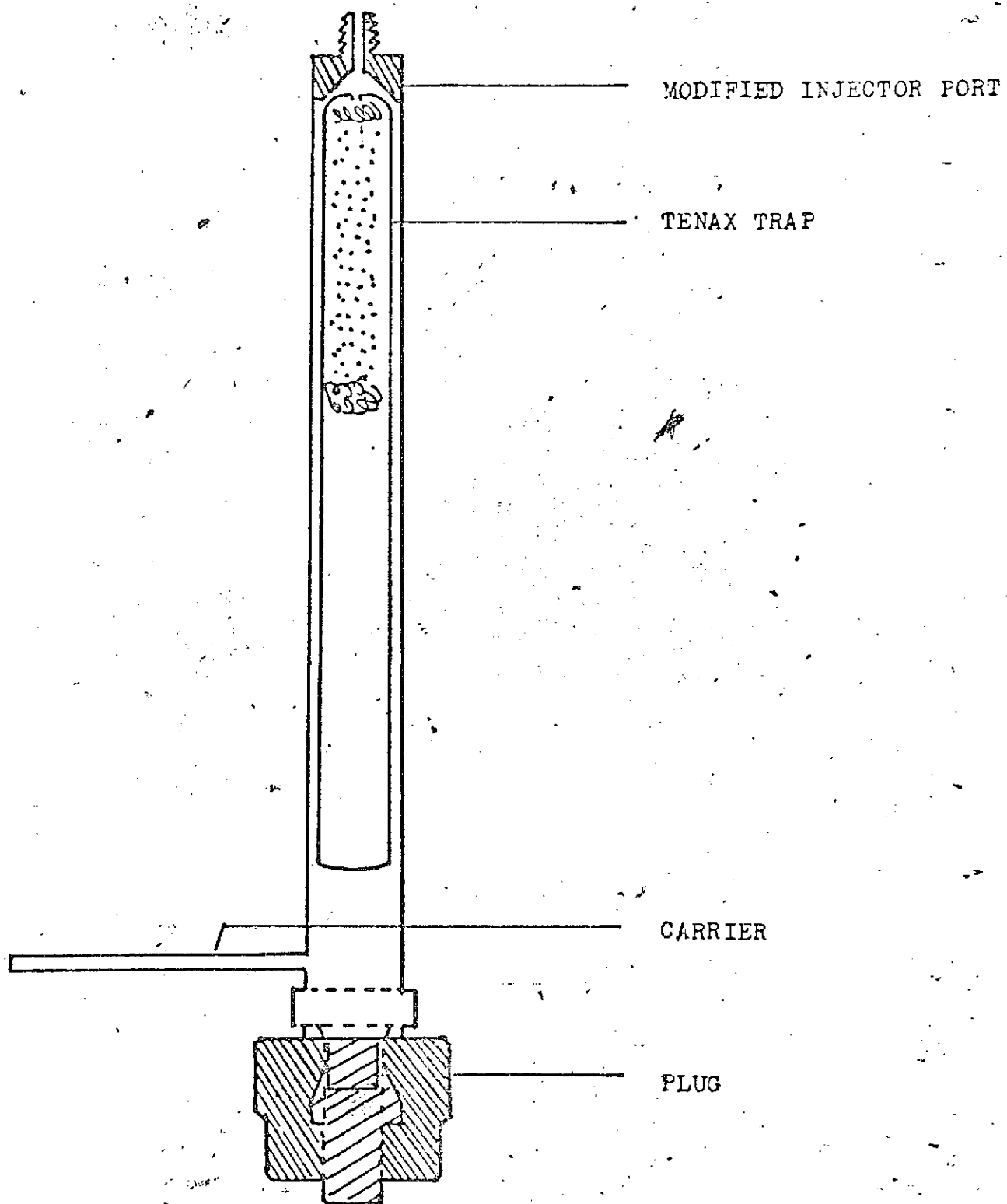
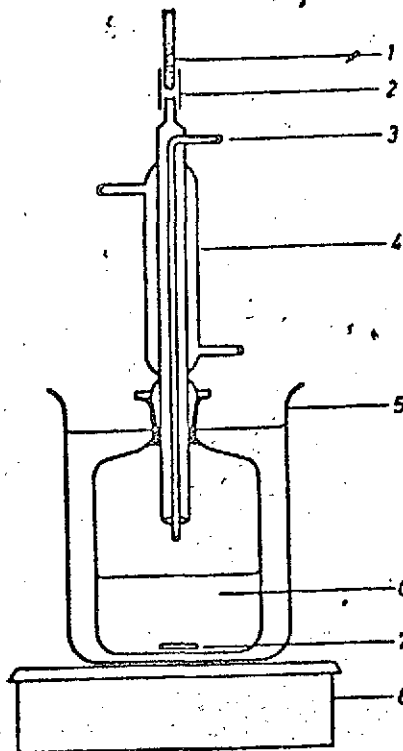


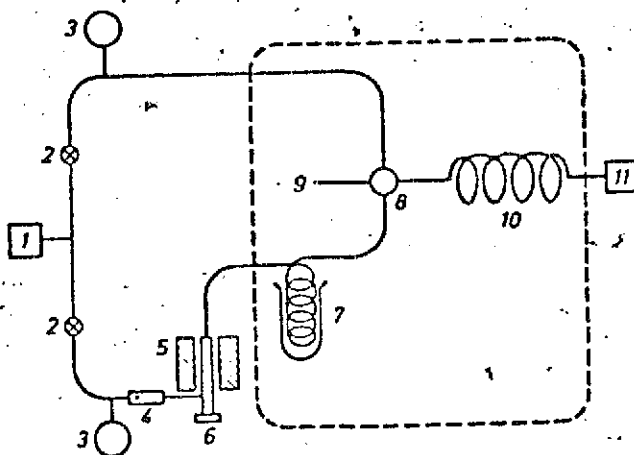
FIGURE 2



2A

• Aqueous Volatile Sampler

1 Trap-insert with Tenax-GC, 2 Teflon sleeve, 3 Helium inlet,  
4 Condenser, 5 Boiling water bath, 6 Sample, 7 Magnetic stirring  
bar, 8 Hot-plate-stirrer



2B

• Sample Analysis and Transfer Flow System

1 Carrier (He) 6 Modified injector port  
2 Teflon sleeve 7 Pre-Column in dry ice  
3 Pressure regulator 8 4-port valve  
4 Rotameter 9 Vent  
5 Injector block 10 Separating column  
11 Detector

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OF POOR QUALITY



from the pre column and a four port valve (Valco Instruments, Houston, Texas), allowing simultaneous carrier flow to the pre column (20 cc/min) and separating column (3 cc/min), was turned. This diverted the sample in the pre column to the separating column to begin the chromatographic separation.

A Perkin-Elmer 900 gas chromatograph (Flame ionization detector) was used for qualitative GC profiles and the injector and detector temperatures were 200°C and 280°C, respectively.

An LKB 9000 combination gas chromatograph-mass spectrometer (LKB-Produkter AB, Bromma, Sweden) was used for identification of significant compounds in the water samples. Sampling, trapping, and GLC conditions were similar to those used on the Perkin-Elmer 900 except the pre column was connected to the separating column manually. The ion source and separator temperatures were 250°C and 220°C, respectively. Analyses were made at 70 eV electron energy. Scanning rate was 4.5 seconds over the mass range 20-350.

### 3.1.3 Quantitation of Volatile Organics

A primary standard at a concentration of 1,250 milligrams per liter (ppm) in water was made for the compounds to be examined. Secondary standards of 50 micrograms per liter (ppb) in water were made by dilution. Fifty milliliters of these secondary standards, representing a total of  $2.5 \times 10^{-6}$  grams of each compound were used for Tenax sampling.

The glassware and Texas traps used were described in the previous section. Glassware was cleaned initially in No-Chromix, sulfuric acid and then rinsed with deionized water and oven dried. The trapping system was assembled and purged with prepurified N<sub>2</sub> passed over Carbosieve B. Fifty

milliliters of the water to be sampled was added to the flask and the flask heated by means of a boiling water bath. The sample was stirred with a magnetic stirring bar and the surface swept at a rate of 20 milliliters per minute with the prepurified  $N_2$ . Initial recoveries were poor (see results section) and refluxing was substituted for this step. The headspace gases were swept through a water condenser prior to entering the Texas trap.

After sampling for 1 hour, the trap was removed and stored in a teflon lined screw cap test tube. The sample was transferred to a dry ice cooled pre column (10' x .05" i.d., ss., coated with DC-200) by placing in a modified injector port and heating for 20 minutes at 200°C, while passing helium gas through the trap and pre column at 20 milliliters per minute. At the end of the desorption period, the pre column was placed in series with an analytical column by means of an eight port switching valve and then flash heated. Gas liquid chromatography was performed on a 5' x 1/8" o.d., s.s. column packed with 5% DC-200, 0.5% Carbowax, 20 M on 100/140 mesh Chromosorb W-HMDS. The temperature was isothermal at 30° C for 2 minutes then programmed to 200°C at 8°C per minute. Carrier gas was helium at 25 milliliters per minute and a flame ionization detector was used.

### 3.2 Preparation of Synthetic Water Samples for Taste Evaluation

Ultrapure pure water was prepared from deionized water by distillation with potassium permanganate in a 43 cm glass fractionating column and stored at 40°F. Atomic absorption analyses showed calcium, magnesium, potassium, and sodium to be present at less than 0.1 ppm each. Volatile organics in the ultrapure water were determined using the Tenax solid adsorbent trapping procedure described in the previous section. A blank

run was made on the cleaned empty apparatus and subtracted from the water sample. The net area of all peaks was multiplied by a calibration factor determined by direct injection of  $C_8$  and  $C_{12}$  hydrocarbons. The results indicated the purified water contained less than 0.2 ppb total volatile organics. Calcium and magnesium ions were added as sulfates and potassium and sodium ions as chlorides to produce water samples with the desired concentrations for taste evaluation.

## 4.0 EXPERIMENTAL RESULTS AND DISCUSSION

### 4.1 Evaluation of Waste Water Reclamation Systems

Product water samples and starting materials from several prototype reclamation systems were chemically analyzed and tasted. Additionally a commercial bottled water, distilled water, and tap water were analyzed and tasted for comparison.

#### 4.1.1 Inorganic Chemical Constituents, Dissolved Gases and Organic Carbon

Four different water samples including two samples from water reclamation pilot systems (Skylab and SWRI), a sample of synthetic water supposedly equivalent to spring water (Foremost) and Houston tap water were analyzed. These analyses included only those factors which we considered most important to palatability (see Table 2). The results of these analyses are given in Table 3. Values for all factors were not obtained for the SWRI sample because of lack of sufficient sample. The relative palatability or taste of the samples was determined by a single taster and is also given (1 is the best tasting water).

The anion and cation values for the Skylab and SWRI samples are very low, as they should be since the reclamation process is intended to remove them. The Foremost sample was also processed to remove all cations and anions, but  $\text{Ca}^{++}$ ,  $\text{Mg}^{++}$ ,  $\text{K}^+$  and  $\text{Na}^+$  were added back to the processed water to enhance the taste. The high  $\text{Cl}^-$  and  $\text{SO}_4^{=}$  result from the addition of the cations as the  $\text{Cl}^-$  and  $\text{SO}_4^{=}$  salts. The organic carbon values are quite high for the SWRI sample. Possible sources of this carbon are discussed in the next section.

TABLE 3  
WATER ANALYSES RESULTS

	<u>SKYLAB</u>		<u>SWRI</u>		<u>FOREMOST</u>		<u>TAP WATER</u>	
Ca <sup>++</sup>	<	1 ppm	<	1 ppm	40	ppm	29	ppm
Mg <sup>++</sup>	<	0.1 ppm	<	0.1 ppm	9.6	ppm	6.2	ppm
K <sup>+</sup>	<	1 ppm	<	1 ppm	1.3	ppm	97*	ppm
Na <sup>+</sup>	<	1 ppm	<	1 ppm	10	ppm		
ACIDITY (as CaCO <sub>3</sub> )		27 ppm		19 ppm	4	ppm	22	ppm
Cl <sup>-</sup>		7 ppm		9 ppm	82	ppm	53	ppm
F <sup>-</sup>		0.4 ppm		—	1.7	ppm	0.6	ppm
NO <sub>3</sub> <sup>-</sup>	<	0.1 ppm		—	<	0.1 ppm		
SO <sub>4</sub> <sup>=</sup>		5 ppm	<	5 ppm	45	ppm	6	ppm
HCO <sub>3</sub> <sup>-</sup> + CO <sub>3</sub> <sup>=</sup>	<	1 ppm	<	1 ppm	<	1 ppm	276	ppm
pH		3.7 ppm		4.5 ppm	4.7	ppm	7.8	ppm
NH <sub>3</sub>	<	0.02 ppm		—	<	0.02 ppm	<	0.02 ppm
DISSOLVED O <sub>2</sub>		3.8 ppm		4.5 ppm	3.0	ppm	5.2	ppm
DISSOLVED CO <sub>2</sub>	<	1 ppm	<	1 ppm	<	1 ppm	<	1 ppm
TOC (Total organic carbon)		1 ppm		23 ppm	<	1 ppm	<	1 ppm
POC (Particulate organic carbon)		0 ppm		1 ppm	0	ppm	0	ppm
DOC (Dissolved organic carbon)		1 ppm		22 ppm	<	1 ppm	<	1 ppm
RELATIVE PALATABILITY		3		3	1		2	ppm

\*K<sup>+</sup> + Na<sup>+</sup>

It can be seen that the better tasting sample (Foremost) is also the sample which better fits the criteria for palatability (see section 5.0). One could speculate that the high organic carbon content of the SWRI sample may have been responsible for the lower relative palatability of this sample, but the lack of important (to palatability) cations and anions may also be an important factor.

#### 4.1.2 Volatile Organic Profiles

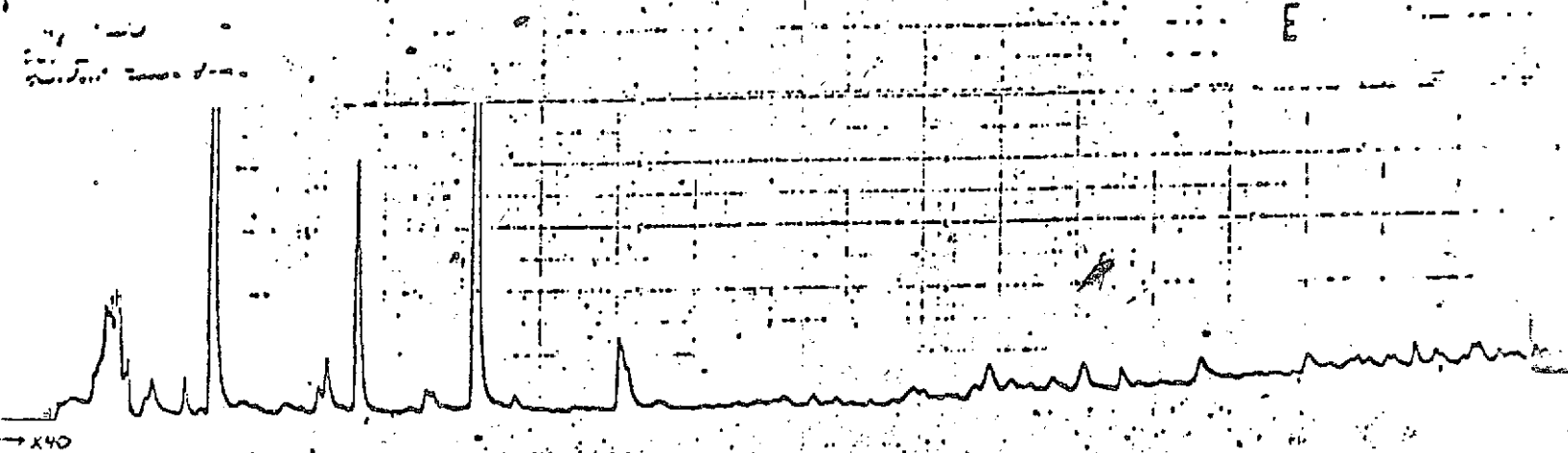
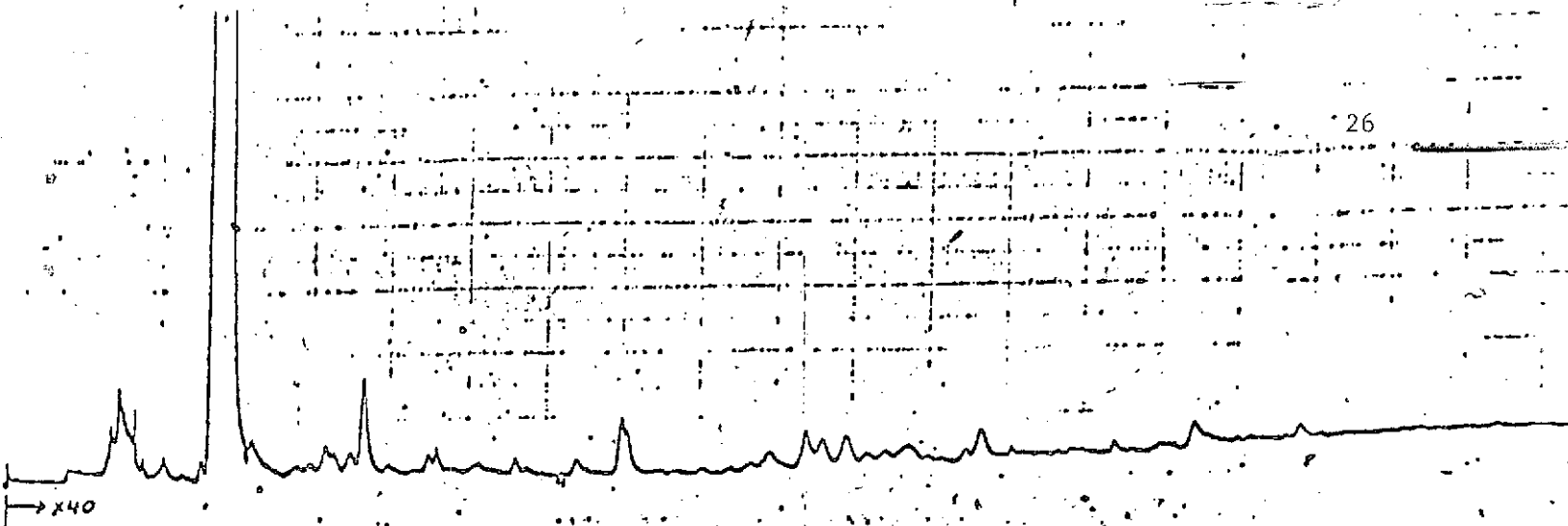
A first step in obtaining waste material contaminants is the determination of volatile organic compounds, because of the high probability of their presence in product water of some reclamation systems (e.g., distillation). Over two hundred volatile organic compounds in human urine have been concentrated, and analyzed by high resolution gas chromatography and at least eighty (80) of these compounds have been identified by combined gas chromatography-mass spectrometry (GC-MS). There is good indication that many of these eighty compounds are indigenous to all human urine. Therefore, in the chemical evolution of waste water reclamation systems, the quality of product water may be more adequately described in terms of efficiency of removal and origin of contamination.

Prior to sampling product water and its starting materials, system blanks and controls were undertaken. Figure 3A represents a chromatographic analysis of a conditioned Tenax trap desorbed and cryogenically transferred to the chromatographic column. Since no sample was passed over the adsorbent, any ensuing peaks would have arisen in the sampling and analytical system. Figure 3B represents the analysis of approximately 30 grams of  $(\text{NH}_4)_2\text{SO}_4$  used as a salting out agent. Figure 3C depicts a deionized water

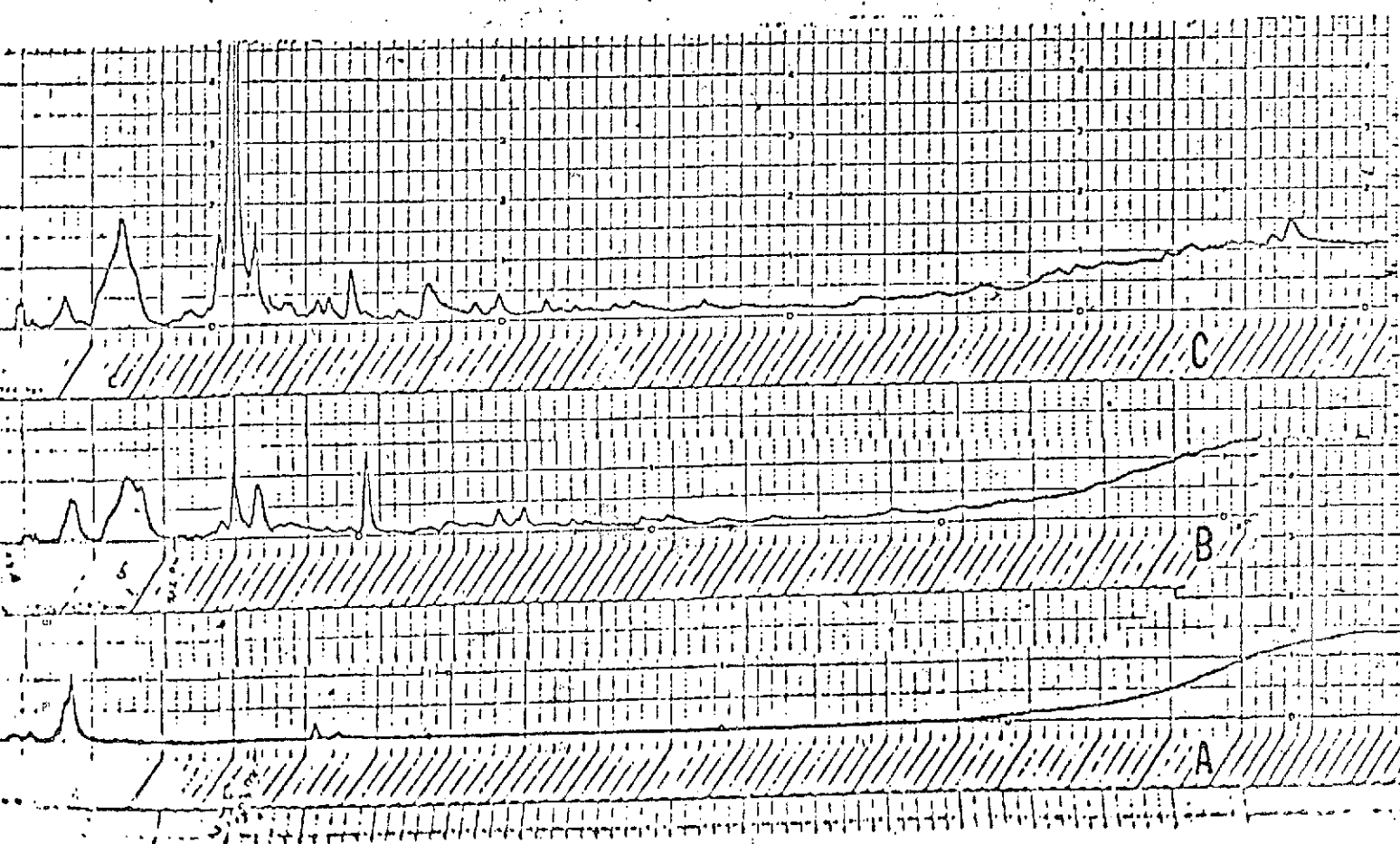
FIGURE 3

VOLATILE ORGANIC PROFILES - CONTROLS

- A. Tenax GC - blank
- B.  $(\text{NH}_4)_2\text{SO}_4$  - blank
- C. Deionized water - control
- D. Distilled water - control
- E. Houston, Texas ground water



Distal Med H<sub>2</sub>O 200mV  
Standard Trace Run





sample, containing 30%  $(\text{NH}_4)_2\text{SO}_4$  as all future aqueous samples do. Figures 3D and 3E respectively represent distilled and Houston, Texas ground water.

The first product water sample examined in a preliminary analysis was from Chemtrix Corporation. Figures 4A and 4B compare the product water and a Houston ground water sample. The striking difference in volatile organic profiles can not be explained in terms of the origin of these organics, since no starting material (urine) was available for comparison.

The first gas chromatographic-mass spectrometric analyses were run on a product water from a General Electric -AEC system using radioisotopes for thermal energy (RITE). The GE-RITE analysis is shown in Figure 5. The similarity of this sample and the Chemtrix sample may be accounted for in part if urine were a starting material. For example, a list of volatile organics found in the GE-RITE sample (Table 4) indicate that some of these compounds have been found in human urine.

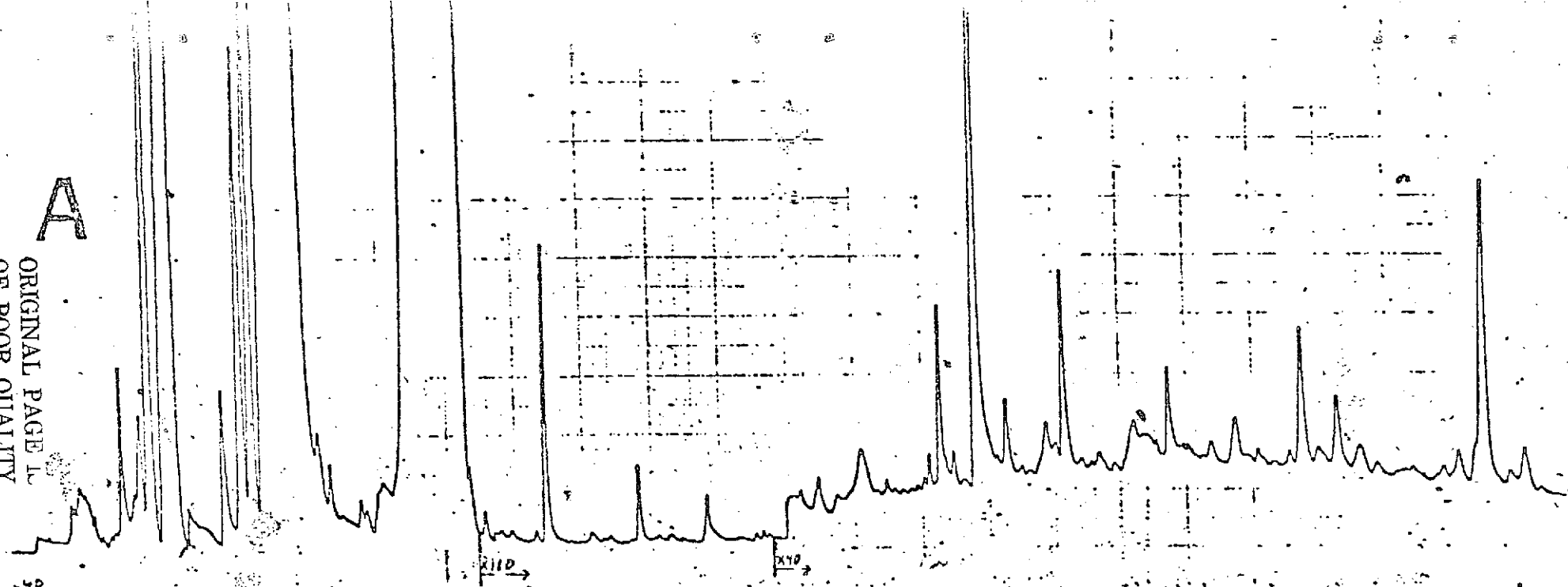
Figure 6 represents the analysis of a commercially bottled water (Foremost), and several major peaks have been identified by gas chromatography-mass spectrometry (Table 4); however, the origin of these compounds is not known. Table 4 also gives the relative total volatile organics found in these samples compared to the Houston ground (tap) water. It can be seen that these values do correlate with taste, the poorer tasting waters being higher. Based on the dissolved organic contents given in Table 3 the upper limit of volatile organics in the poor tasting Skylab water sample is 1 ppm or 1000 ppb. This can then be taken as a maximum allowable limit for the total volatile organics. Individual components may

FIGURE 4

VOLATILE ORGANIC PROFILES IN A POTABLE WATER SYSTEM

- A. Regenerated Water System - Chemtrix Corporation
- B. Houston, Texas ground water

**A**  
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**B**

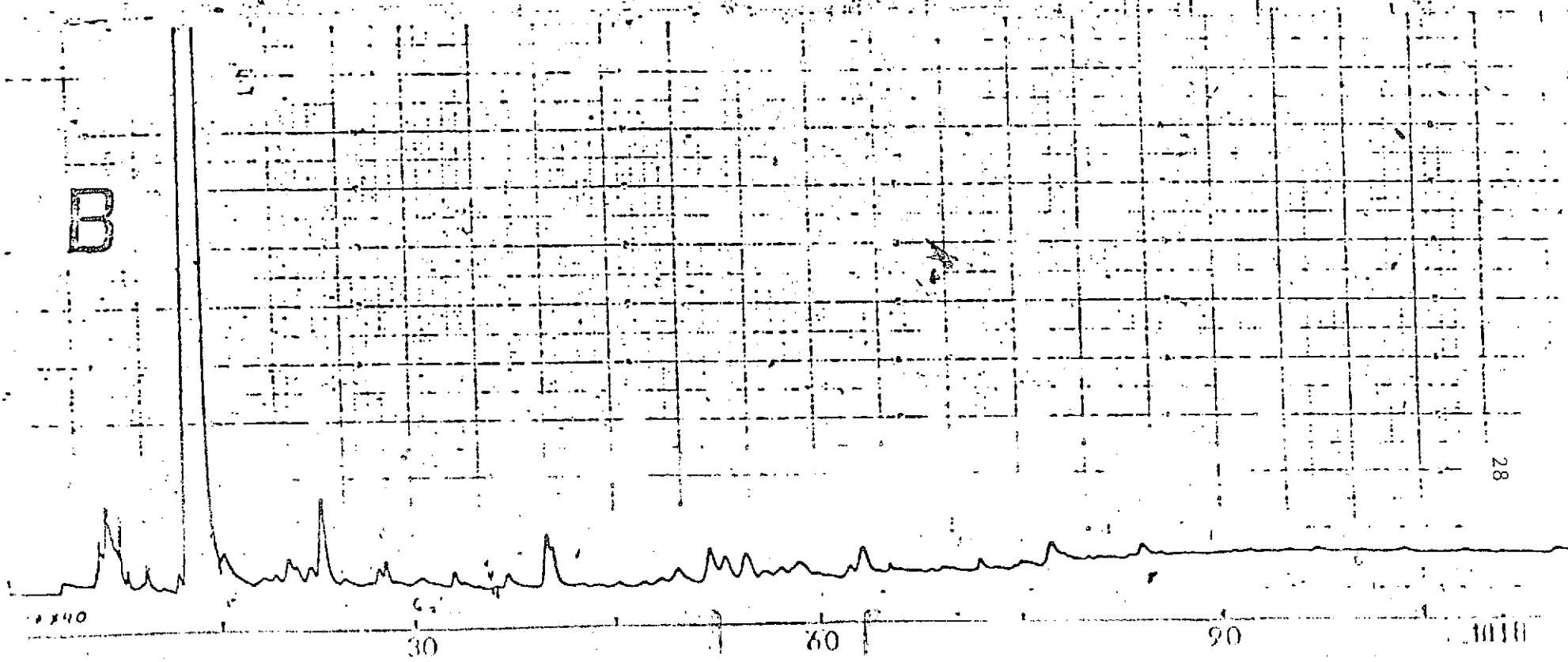
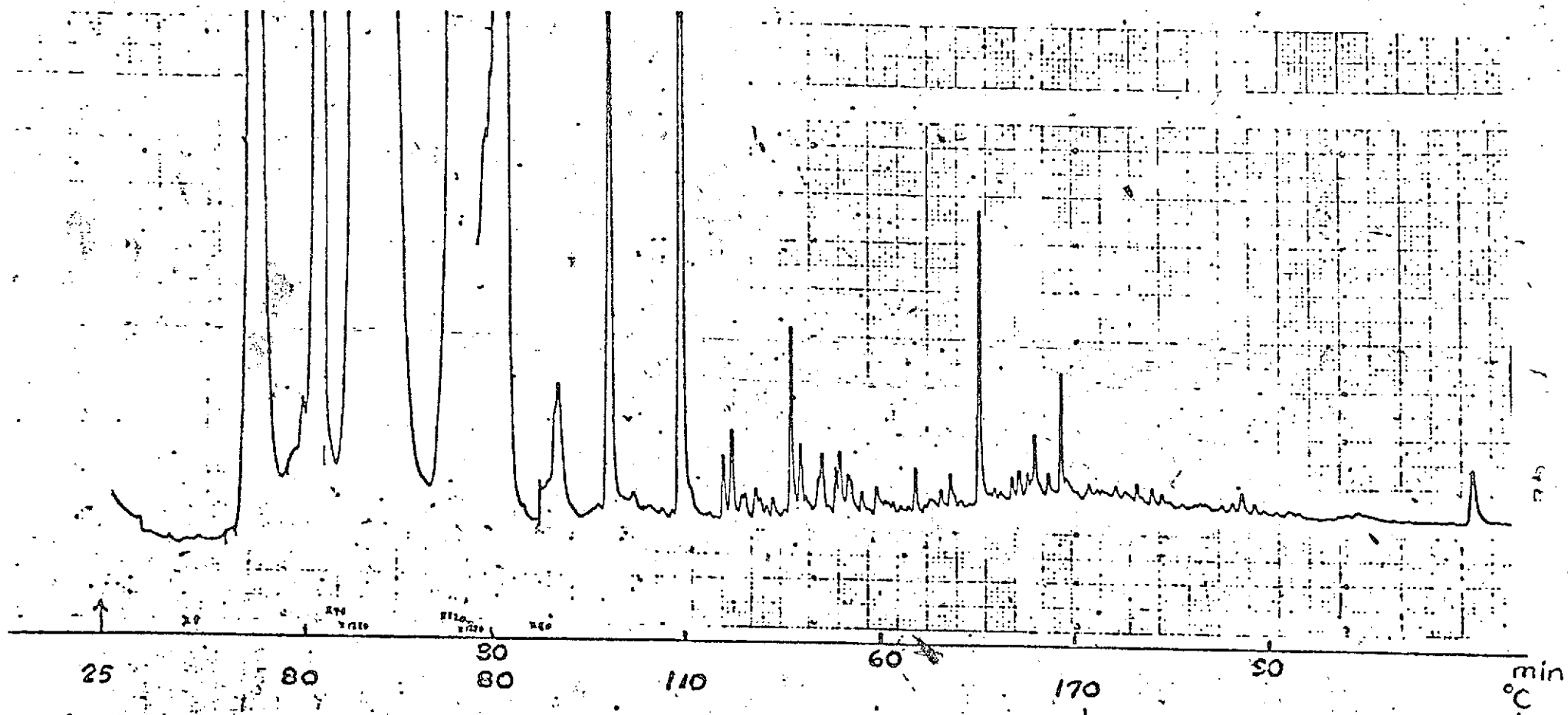


FIGURE 5

VOLATILE ORGANIC COMPOUNDS IN A REGENERATED  
WATER SYSTEM (GE-RITE)



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TABLE 4

VOLATILE ORGANICS\*  
IN POTABLE WATER

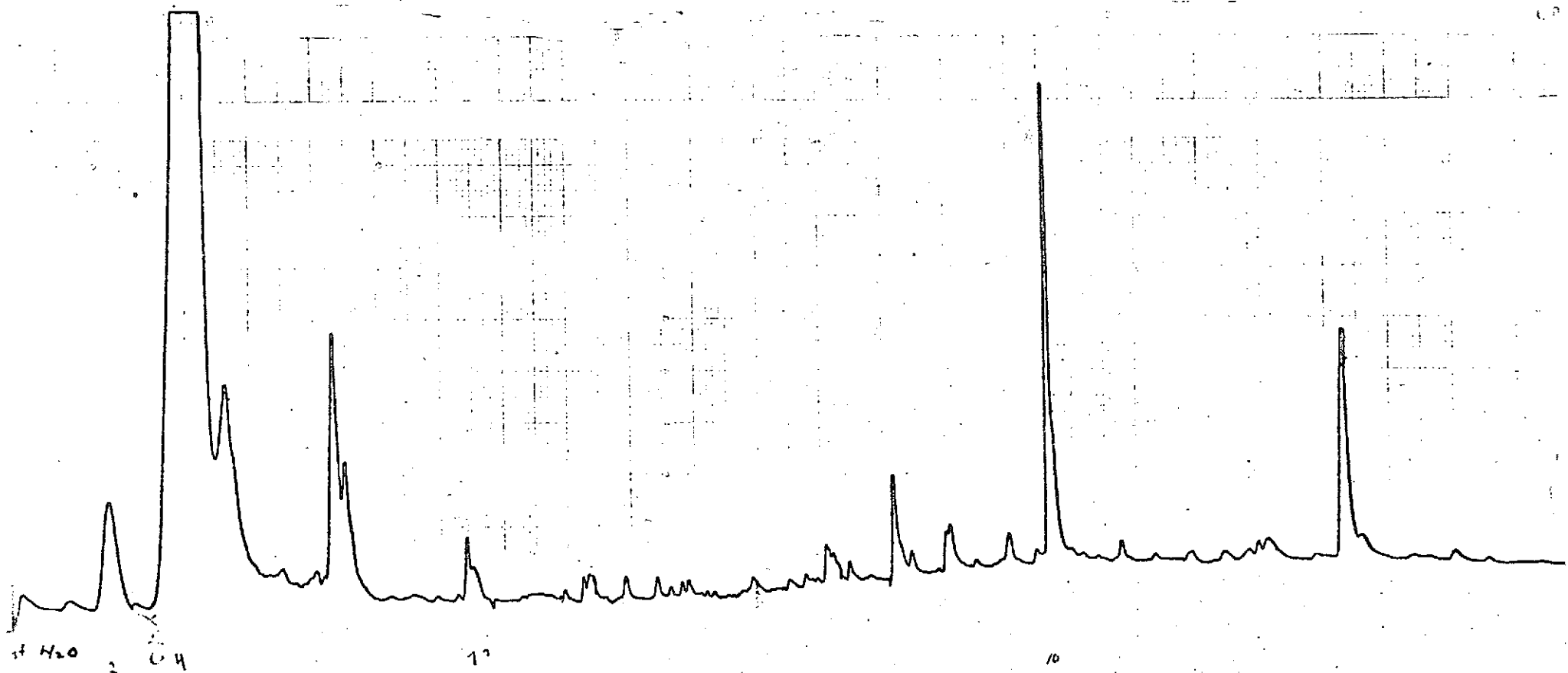
SKYLAB	GE	SWRI	FOREMOST
	Acetone**		
	2-Butanol**		
Undecane	Benzene	High MW's	Dichloromethane
	Pentanone**		Benzene
Cyclohexane	Dioxane	Dioxane	Undecane
	Isopropanol**	2-Methyl-1,3 dioxalane	
Silicones	Toluene		Naphthalene
	Diethylsulfide**		
Dodecane	n-C <sub>10</sub>		
	Propanol**		
	Methyl propanol		
	3-methyl-1-butanol		
	n-C <sub>11</sub>		
	Trimethyl benzene		
TOTAL VOLATILE ORGANIC CONTENT RELATIVE TO TAP WATER			
100	10,000	100	10

\*in order of elution

\*\*previously found in human urine

FIGURE 6

VOLATILE ORGANIC PROFILE OF A COMMERCIALY  
AVAILABLE BOTTLED WATER (FOREMOST)



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require control to 1-10 ppb levels, however, depending on their odor threshold and potential toxicity. A sample of Skylab water was profiled for volatile organics and the results are shown in Figure 7. This water does not appear to have a profile of a urine distillate as the previous systems and the compounds identified may indicate contaminants arising from the system and/or storage containers.

Figure 8A, B, and C compare raw urine, treated urine (BioPal VRO-20;  $\text{H}_2\text{SO}_4$ ; Dow Corning antifoam) and product water regenerated from treated urine, respectively (Southwest Research Institute). This type of comparison is preferred for the evaluation of regeneration systems and can be used for the determination of sources of the contaminants. Based on retention times alone (since GC-MS was used only for the product water) a general comparison may be made between these chromatograms. Peaks numbered in Figure 8B not appearing in the starting urine could have come from the additives and, even after regeneration, peak number 1 is found in the product water (Figure 8C). Although the product water appears to be devoid of many urine volatiles, new compounds appeared in addition to those found in the treated urine.

#### 4.2 Quantitation of Volatile Organics

The results of the qualitative volatile organic profile work previously described combined with the knowledge of organoleptic sensitivities indicated the need for quantitating volatile organic compounds in water to the low ppb concentration level. The success of the Tenax solid adsorbent sampling and analysis procedure in qualitative work led us to select this technique for quantitative development.

FIGURE 7

VOLATILE ORGANIC PROFILE OF SKYLAB WATER

NA-0-140  
7-11-73

X160

0.001

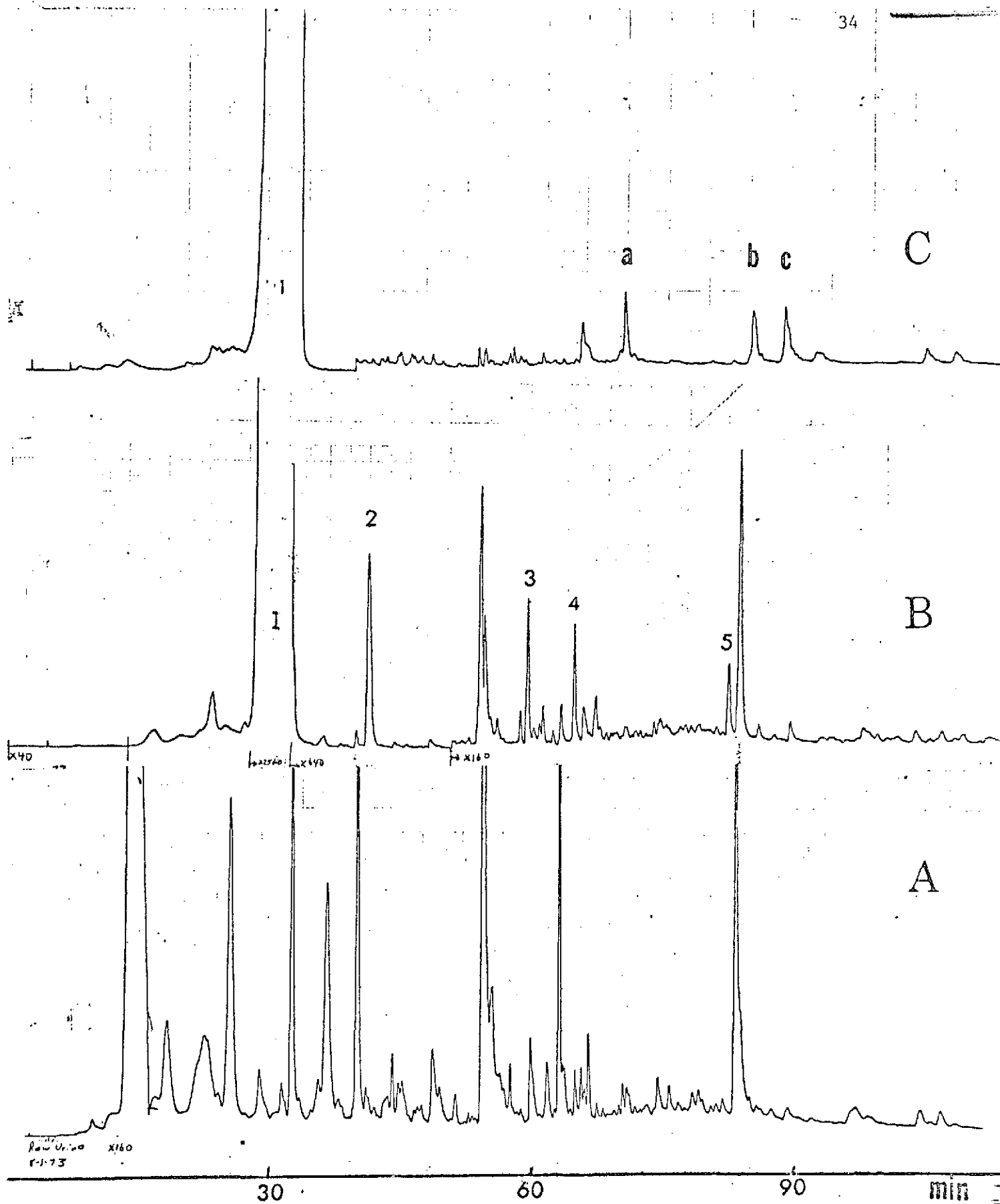
5 7 9 10

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FIGURE 8

COMPARISON OF VOLATILE ORGANIC PROFILES  
(SOUTHWEST RESEARCH INSTITUTE)

- A. Raw Urine
- B. Treated Urine
- C. Product Water



#### 4.2.1 Discussion

For the Tenax procedure to be of general use it must be capable of sampling organic compounds of differing polarity, volatility, dissociation, and chemical stability. In this particular application compounds indigenous to human urine or degradation products of urine metabolites were of primary interest.

With these thoughts in mind the following four compounds were chosen for evaluation of the quantitative reproducibility and sensitivity:

2-butanol	$\begin{array}{c} \text{OH} \\   \\ \text{CH}_3\text{CH}_2\text{CHCH}_3 \end{array}$	b.p. 100°C
p-dioxane	$\begin{array}{c} \text{CH}_2-\text{CH}_2 \\   \quad \quad   \\ \text{O} \quad \quad \text{O} \\   \quad \quad   \\ \text{CH}_2-\text{CH}_2 \end{array}$	b.p. 101°C
4-methyl-2-pentanone	$\begin{array}{c} \text{O} \quad \quad \text{CH}_3 \\    \quad \quad   \\ \text{CH}_3-\text{C}-\text{CH}_2-\text{CH}-\text{CH}_3 \end{array}$	b.p. 117°C
pyrrole	$\begin{array}{c} \text{CH} \quad \quad \text{NH} \\   \quad \quad   \\ \text{CH} \quad \quad \text{CH} \\   \quad \quad   \\ \text{CH} \end{array}$	b.p. 131°C

These compounds show partial to very good solubility in water, varying degrees of dipole moment, and a boiling point range which makes simple distillation from a water matrix difficult. In addition, all of these compounds are known to be present in human urine, having been observed in product water from urine reclamation systems (Table 4). Vigorous conditioning of the Tenax traps (24 hours at 225°C) removed all interfering artifacts for the compounds of interest. Sampling system blanks showed

background to be less than  $10 \times 10^{-9}$  grams. Blanks from the deionized water used for preparing the secondary standard however showed a large number of interferants at levels greater than 1 ppm. It was necessary to boil the DI water with hydrogen peroxide in order to reduce these contaminants. This reduced interference with 2-butanol, 4-methyl-2-pentanone, and pyrrole to less than .2 ppb. However, p-dioxane interference was reduced to only 6 ppb.

Recovery tests, using the spiked standards, as described in 3.1.3 were initiated. Initial recovery for p-dioxane was less than 10% and less than 4% for 2-butanol, 4-methyl-2-pentanone, and pyrrole. Since injections of these standards directly onto a Tenax trap showed negligible loss of sample, it was felt that the compounds were not being volatilized from the aqueous phase. Tests were rerun eliminating the water bath for heating in favor of refluxing.

Figure 9 is a chromatogram of a direct injection containing  $2.5 \times 10^{-6}$  grams each of the four compounds. Figure 10 shows a typical sampling system blank (note the lower attenuation) and Figure 11 is a chromatogram of a 50 ppb spiked sample sampled with Tenax. Table 5 presents area response for standardization. Table 6 presents area response for the sampling system blanks. Table 7 shows area response for the recovery tests of samples spiked with 50, 25, and 5 ppb quantities. As can be seen from Table 7, precision calculated at one standard deviation ranges from approximately 10 to 20 percent and recovery from 68 to 88%. The recovery values are plotted in Figure 12 and calibration curves drawn for the four compounds. The linearity and data point spread appear good. The large data point spread of dioxane is probably due to the large and variable blank.

FIGURE 9

DIRECT INJECTION OF FOUR COMPONENT QUANTITATIVE STANDARD



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4-methyl-2-pentanone

pyrrole

p-dioxane

2-butanol

2 $\mu$ l

X 640

FIGURE 10

QUANTITATIVE SAMPLING SYSTEM BLANK

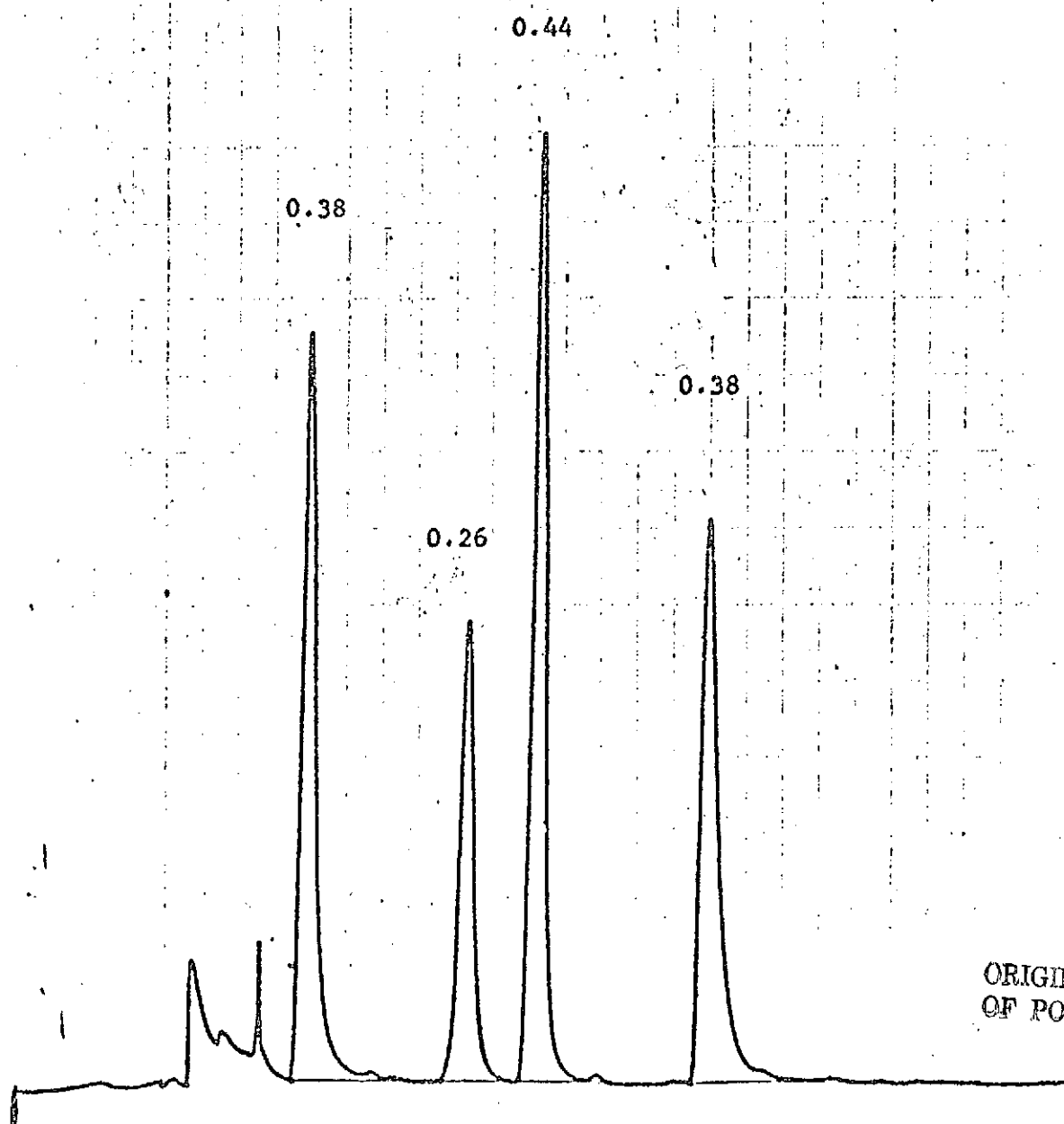
0.48

X 40

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FIGURE 11

TENAX HEADSPACE SAMPLING OF SPIKED WATER SAMPLE



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TABLE 5  
AREA RESPONSE FOR  $2.5 \times 10^{-6}$  gm STANDARDS

Run	2-butanol	p-dioxane	4-methyl-2-pentanone	pyrrole
1	288	160	320	512
2	275	160	288	294
3	275	154	282	294
4	301	186	294	294
5	282	186	294	294
Average	282	166	301	301

TABLE 6  
AREA RESPONSE FOR SAMPLING SYSTEM BLANKS

Run	2-butanol	p-dioxane	4-methyl-2-pentanone	pyrrole
1-20	-	18.8	-	-
3-15	-	12.4	-	-
1-22	-	19.2	-	-
5-13	-	24.4	-	-
Average	-	18.8	-	-
Calculated as grams		$0.3 \times 10^{-6}$ gms		

TABLE 7  
RECOVERY OF STANDARDS FROM SPIKED SOLUTIONS

Recovery of Standards from 50 Milliliters of 50 ppb Water Solution

Run	2-butanol	p-dioxane	4-methyl-2-pentanone	pyrrole
2-16	237	160	275	262
4-13	256	147	320	275
6-14	-	102	282	198
2-18	262	147	269	250
2-20	243	166	282	243
7-10	275	96	288	256
9-2	211	128	186	198
Average	250	134	269	243
Calculated as grams	$2.2 \pm .2 \times 10^{-6}$	$2.0 \pm .4 \times 10^{-6}$	$2.2 \pm .4 \times 10^{-6}$	$2.0 \pm .2 \times 10^{-6}$
Blank correction	-	$.3 \times 10^{-6}$ gms	-	-
Recovery	88%	68%	88%	80%

TABLE 7 CONTINUED

## RECOVERY OF STANDARDS FROM SPIKED SOLUTIONS

Recovery of Standards from 50 Milliliters of 25 ppb Water Solution

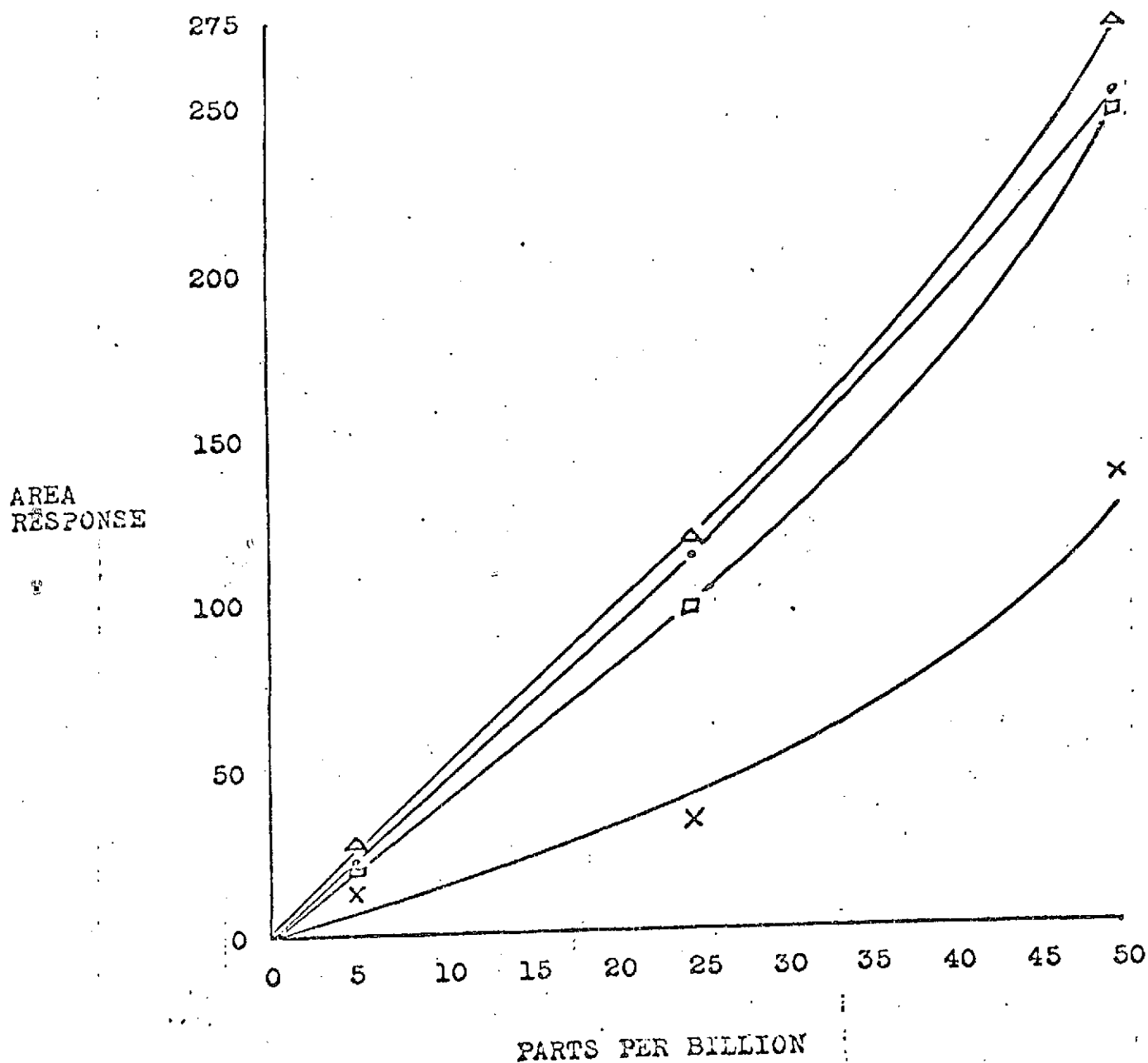
Run	2-butanol	p-dioxane	4-methyl-2-pentanone	pyrrole
1	108	54.4	114	73.6
2	119	59.5	111	113
3	108	58.5	123	108
Average	112	57.5	116	98.2
Blank correction	-	18.8	-	-
Recovery	97%	50%	88%	72%

Recovery of Standards from 50 Milliliters of 50 ppb Water Solution

Run	2-butanol	p-dioxane	4-methyl-2-pentanone	pyrrole
1	23.1	26.4	26.4	12.0
2	25.0	36.0	26.6	27.8
3	25.0	-	27.2	22.0
Average	24.4	31.2	26.7	20.6
Blank correction	-	18.8	-	-
Recovery	107%	80%	100%	74%



FIGURE 12  
RECOVERY OF STANDARDS FROM CONCENTRATIONS ON TENAX 43



- = 2-butanol
- x = p-dioxane
- Δ = 4-methyl-2-pentanone
- ◻ = pyrrolle

### 4.3 Taste Panel Evaluations

Synthetic water samples have been made up and tasted with the objective of establishing the minimum essential ingredients to achieve good taste based on the enhancement factors identified in Table 2. The samples were prepared from ultrapure water to insure that no negative factors were present. Initially three samples of water were made up with the following concentrations (mg/l) of Ca, Mg, K and Na ions:

	Ca	Mg	K	Na
Water #1	≤0.1	≤0.1	≤0.1	≤0.1
Water #2	20	10	0	2
Water #3	40	10	2	10

Total organic volatiles were determined quantitatively by the solid adsorbent trapping and analysis method and verified less than 0.2 ppb for all three matrices. Three tasters were used and samples were tasted at room temperature and 40°F. Two of the tasters did not know which samples they were tasting while one did.

Table 8 presents comparisons of preference and a summation of the times each water was selected in a certain category. Tasters were asked not to describe waters as tasting good or bad but to rank them in order of preference. Tasters I and II made a repeat on a succeeding day to see if any changes were made in preference. Taster I made a reversal in least and better but both tasters selected the same water as best that they had the day before. There is a remarkable difference in taste preference for waters #2 and #3 versus water #1. The ultrapure water was never selected as being best tasting while it was the least desirable seven times. The samples with added electrolytes showed no great difference in preference.

TABLE 8  
PREFERENCE FOR SYNTHETIC WATERS

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TASTE PREFERENCE

Room Temperature (day 1)	Least	Better	Best
Taster I	#3	#1	#2
Taster II	#1	#2	#3
Taster III	#1	#2	#3
40 F (day 1)	Least	Better	Best
Taster I	#1	#3	#2
Taster II	#1	#2	#3
Taster III	#1	#3	#2
Room Temperature (day 2)	Least	Better	Best
Taster I	#1	#3	#2
Taster II	#1	#2	#3

NUMBER OF TIMES A WATER SELECTED IN A CATEGORY

Water #	Least	Better	Best
Water #1	7	1	0
Water #2	0	4	4
Water #3	1	3	4

---

The above test indicated that water with some added ionic constituents is obviously preferable to "zero" pure water. A second test was conducted in an attempt to better define the concentration range of the various anions and cations which produce the best tasting water. Again all samples were made up from water containing less than 0.2 ppb volatile organics, less than 1 ppm total organic carbon, and less than 0.1 ppm of any of the anions and cations to be added; the values for the latter two being the limits of detection. It is necessary to start with water that is both organically and inorganically pure in order to be certain that any taste qualities are truly attributable to the added components. It should be noted also that dissolved gas content was not controlled in these tests but should be very low (less than 0.1 ppm), since the water was purified by distillation.

The water samples for the second taste test were made up to the anion and cation contents given in Table 9. Six different samples were tested one of which (#5) was tap water. The taste panel was made up of six members who were instructed to taste each water individually and state whether it was bad, average, or good tasting. At the conclusion each was asked to select the best tasting water. No attempt was made to remove bias, nor was any attempt made to influence a preference. All samples were tested at room temperature. Evaluations and comments of the tasters are presented in Table 10. As anticipated the waters with high (sample #6) and no (sample #4) electrolyte content were rated objectionable or not as pleasing as others. Since the tap water sample was not highly rated it was not chemically analyzed. It should be noted that the taste panel could not select an

TABLE 9  
CHEMICAL COMPOSITION OF SYNTHETIC SAMPLES FOR TASTE EVALUATION

	#1	#2	#3	#4	#5	#6
$\text{Ca}^{++}$	20	25	15	0.1	T	40
$\text{Mg}^{++}$	20	25	7.5	0.1	A	40
$\text{K}^{+}$	10	5	1	0.1	P	20
$\text{Na}^{+}$	10	5	5	0.1	(well)	20
$\text{SO}_4^{=}$	40	50	15	0.1	W	80
$\text{Cl}^{-}$	35	43	26	0.1	A	70
$\text{NO}_3^{-}$	69	74	1.6	0.1	T	122
$\text{HCO}_3^{-}$	28	14	14	0.1	E	28
					R	

TABLE 10

## TASTE PANEL EVALUATION OF SYNTHETIC WATER SAMPLES

Sample Number	Taster Comments		
1	(1) Hard, like apartment water (4) Good tasting	(2) Good tasting (5) Good tasting	(3) Good tasting (6) Good
2	(1) Less hard than #1, all right (4) Good tasting	(2) Not as good as #1, but still good (5) Did not like	(3) Not as good as #1, but still good (6) Slightly saline
3	(1) Similar to #1 and #2 (4) Good tasting	(2) Good tasting (5) Good tasting	(3) Good tasting (6) Pleasing
4	(1) Do not like at all (4) Bad tasting	(2) Bad tasting (5) Better than #2 or #3	(3) Bad tasting (6) Bad tasting
5	(1) Best one (4) Mineral or iron taste	(2) Same as #2 (5) Left film on tongue	(3) Mineral or iron taste (6) Medicinal flavor
6	(1) Similar to #4, bad (4) Flat tasting	(2) Not as good as #2, but drinkable (5) OK	(3) Good, but not as good as #1 (6) Left an after-taste

(Taster number)

obvious best sample and that samples #1 and #3 were generally equally good. Based on these results it is felt that the following salt concentrations should be added to product water from water reclamation systems for further taste evaluations; with the provision that a portion of either the  $K^+$  or  $Na^+$  may later be added as a fluoride for physiological reasons.

$Ca^{++}$	20 ppm (as $CaCl_2$ )
$Mg^{++}$	10 ppm (as $MgSO_4$ )
$K^+$	2 ppm (as $KCl$ )
$Na^+$	10 ppm (as $NaCl$ )

## 5.0 CONCLUSIONS AND RECOMMENDATIONS

### 5.1 Spacecraft Water Quality-Palatability Specifications

The principal areas which must be addressed in any set of spacecraft water quality-palatability specifications are summarized below:

- (1) Toxicity
- (2) Physiological requirements
- (3) Psychological aspects
- (4) Appearance
- (5) Palatability

Toxic chemical constituents to be included must be related to the particular spacecraft and water system as well as the duration of the mission. If the water system is regenerative, the raw material source (e.g., urine and/or faecal matter) must be considered since compounds not efficiently removed by the regeneration process could build up to potentially toxic levels. Exogenous sources of potentially toxic compounds (e.g., spacecraft outgassing) could also be concentrated in the drinking water if they are not efficiently removed.

The question of physiological requirements was discussed with Dr. Malcolm Smith, Branch Chief, Food and Nutrition Branch, NASA-JSC. It was agreed that all mineral balance and trace element deficiencies would be compensated for in the food supplies. Any adjustments required to include the contribution from the water supply will be made at a later date when the chemical definition of the water is completed.

Psychological aspects involving consumption of regenerated or reclaimed water will require the user to be educated in the design and operation of the system.



Values have been established for the factors which determine appearance and palatability. These values are given in Table 11 and can serve as a basis for any further evaluation of palatability factors. The values given for color and total solids are perhaps superfluous as it is difficult to imagine these values being above specified limits if all other specifications are met. The values for inorganic chemical constituents reflect the limited taste panel studies conducted in this study and are valid only if the organic constituents are below the specified levels. No value can be set for single volatile organic components until more quantitative information becomes available on the effect of various organic compounds. This specification need concern only those compounds found to be associated with a particular water system and should also consider any toxicity problems which such compounds may present. This specification also lists several chemical constituents and other properties which are thought to be important for water palatability but have not yet been evaluated. It is not known which of these factors are actually essential for good tasting water and whether there are synergistic or antagonistic effects for various combinations of these factors. Such knowledge is essential in order to establish final palatability criteria. A detailed examination of these palatability factors should be undertaken in future work.

## 5.2 Evaluation of Spacecraft Water Reclamation Systems

The results of inorganic, nonvolatile organic, and volatile organic profile analysis of reclaimed water samples completed during this study indicate that nonvolatile and volatile organic compounds are not

TABLE 1.1

## SPACECRAFT WATER QUALITY-PALATABILITY SPECIFICATIONS

## \*APPEARANCE

Color -  $\leq 5$  on cobalt scale

Total solids - less than 50 ppm

## \*PALATABILITY

Dissolved gases

 $\text{CO}_2$ : 1-5 ppm $\text{O}_2$ : 1-5 ppm

Chemical Constituents - Inorganic

 $\text{Ca}^{++}$ :  $20 \pm 5$  ppm $\text{Cl}^-$ :  $30 \pm 10$  ppm $\text{Mg}^{++}$ ,  $\text{Na}^+$ :  $10 \pm 2$  ppm $\text{SO}_4^{=}$ ,  $\text{NO}_3^{=}$ :  $40 \pm 10$  ppm $\text{K}^+$ :  $2 \pm 1$  ppm $\text{HCO}_3^{=}$ ,  $\text{CO}_3^{=}$ :  $10 \pm 5$  ppm $\text{Cl}^-$ :  $30 \pm 10$  ppm $\text{SO}_4^{=}$ ,  $\text{NO}_3^{=}$ :  $40 \pm 10$  ppm

Chemical Constituents - Organic

Nonvolatile

Total Organic Carbon (TOC):  $\leq 1$  ppmDissolved Organic Carbon (DOC):  $\leq 1$  ppmParticulate Organic Carbon (POC):  $\leq 1$  ppm

Volatile

Total Headspace Extractable: 1 ppm

Single Headspace Extractable: To be determined

removed to the low concentration levels consistent with palatability. These results have been somewhat confused by the lack of contamination control in the sampling and sampling handling procedures used to examine these pilot reclamation systems; however the need for an independent evaluation of potential reclamation systems has been clearly established.

The preliminary results obtained in evaluating the ability to quantitate volatile organics with the Tenax solid adsorbent trapping and analysis procedure are very encouraging. It is apparent that this technique has a very high potential in the future evaluation of spacecraft water reclamation system, and should be exploited to the fullest possible extent.

An effort should be made to evaluate the prototype water reclamation systems selected for future use in spacecraft by working with the organization operating the prototype system to establish proper sampling and sample handling procedures; and to perform analysis of such samples for inorganic, nonvolatile organics, and volatile organics which effect palatability as defined in the palatability specifications developed during this program (see Table 11). The attainment of qualitative and quantitative data on specific organic compounds may provide extremely valuable information related to palatability and toxicity and will provide a basis for determining if any in-flight monitoring is necessary. It is clear that a concern for accepting palatability cannot be separated from the evaluation of regeneration systems in terms of the presence of potentially toxic compounds which may constantly be recycled (and therefore concentrated) in a spacecraft environment. Once these potential toxic and unpalatable organics are known to be removed, suitable inorganics may then be added for good taste.

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## 7.0 SUMMARY

The principal factors affecting water quality and palatability are the presence of dissolved gases, the concentration of various inorganic cations and anions and the organic carbon content. Organic carbon can be differentiated as nonvolatile and volatile organic matter. The latter is of greater significance in palatability considerations since both taste and odor contribute to palatability. Volatile organic compounds present in parts per billion (ppb) concentrations in water can have negative effects on palatability and may also affect water quality from the standpoint of toxicity. A new solid adsorbent trapping and analysis system has been applied to the qualitative analysis of volatile organic compounds in product water of several spacecraft water reclamation systems. Conventional atomic adsorption analyses for the palatability related inorganic constituents were also carried out. The results indicated that organic constituents were not removed efficiently and may be responsible for the poor taste of these waters. The solid adsorbent system was further developed for quantitation of organic volatiles and shown capable of quantitation at the 5-50 ppb level. This technique was used to verify that the volatile organic content of synthesized water samples was sufficiently low to not contribute negative palatability. Inorganic constituents were added to the ultrapure water and the resultant samples evaluated by a taste panel. The results of these taste tests and the other information above have been incorporated into a specification for spacecraft water quality-palatability. The application of the solid adsorbent trapping and analysis system to the evaluation of the water reclamation system



chosen for future spaceflights can greatly enhance our ability to further define spacecraft water criteria.

## 8.0 APPENDIX

## 8.1 List of Figures

Figure No.	Title	Page
1	Tenax Trap and Modified Injector Port	18
2	A. Aqueous Volatile Sampler	19
	B. Sample Analysis and Transfer Flow System	
3	Volatile Organic Profiles - Controls	26
4	Volatile Organic Profiles in a Potable Water System	28
5	Volatile Organic Profiles in a Regenerated Water System (GE-RITE)	29
6	Volatile Organic Profile of a Commercially Available Bottled Water (Foremost)	31
7	Volatile Organic Profile of Skylab Water	33
8	Comparison of Volatile Organic Profiles of Raw Urine, Treated Urine and Product Water	34
9	Direct Injection of Four Component Quantitative Standard	37
10	Quantitative Sampling System Blank	38
11	Tenax Headspace Sampling of Spiked Water Sample	39
12	Recovery of Standards from Concentrations on Tenax	43

## 8.2 List of Tables

Table No.	Title	Page
1	Comparison of Water Standards	8
2	Palatability Related Factors	14
3	Water Analysis Results	24
4	Volatile Organics in Potable Water	30
5	Area Response for $2.5 \times 10^{-6}$ g Standards	40
6	Area Response for Sampling System Blanks	40
7	Recovery of Standards from Spiked Solutions	41
8	Preference for Synthetic Water Samples	45
9	Chemical Composition of Synthetic Samples for Taste Evaluation	47
10	Taste Panel Evaluation of Synthesized Water Samples	48
11	Spacecraft Water Quality-Palatability Specifica- tions	52